Simulation Studies on Some Nearest Neighbor Rules for Statistical Classification.[1]

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David Aarons and Somesh Das Gupta

University of Minnesota

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1. Introduction. The two-population classification problem is to identify a population π_0 with one of two given populations π_1 and π_2 based on observations from these populations on a random vector X. We shall consider here X to be univariate. Let F_i be the c.d.f. of X in π_i $(i = 0, 1, 2)$. Thus our problem is to test $H_1: F_0 = F_1$ vs. $H_2: F_0 = F_2$. In this paper we have considered some rules which are suggested in the literature when F_1, F_2 are not known except that they are continuous. We have studied the performances of the following three rules by simulation.

Let X_0, X_{1i} $(i = 1,\ldots,n_1)$, X_{2i} $(i = 1,\ldots,n_2)$ be random observations on X from the populations π_0, π_1, π_2, respectively.

Rule I. 1-NN (nearest neighbor) Rule: Measure distances of X_0 from X_{1i}'s and X_{2i}'s and based on these distances classify X_0 into the population to which its nearest neighbor belongs.

Rule II. 1-RNN (rank nearest neighbor) Rule: Pool all the observations and order them.

(a) If X_0 is the largest or the smallest observation classify X_0 into the population of its nearest neighbor (based on ranks).

(b) If both the right-hand and the left-hand nearest neighbor of X_0 (denoted by U_1 and V_1) belong to the same population, classify X_0 into that population.

(c) If U_1 and V_1 belong to different populations classify X_0 into π_1 and π_2 with probabilities 1/2 and 1/2, respectively. (We call this case a "tie".)

Rule III. 2-RNN Rule: Apply the 1-RNN rule. If a tie occurs, delete the observations corresponding to U_1 and V_1 and apply the 1-RNN rule again on the remaining observations.

The first rule was suggested and studied by Fix and Hodges (1951, 1953). DasGupta and Lin (1977) proposed the RNN rules and obtained the asymptotic probabilities of misclassification as $n_1, n_2 \to \infty$. For a given rule δ, let its PMC under $F_0 = F_1$ be given by

$$\alpha(\delta) = Pr[\delta \text{ classifies } X_0 \text{ into } \pi_2 \,|F_0 = F_1] .$$

Let $\alpha_1^*, \alpha_2^*, \alpha_3^*$ be the asymptotic values of α corresponding to the above rules 1, 2 and 3. Let f_i be the p.d.f. of F_i with respect to Lebesgue measure $(i = 1,2)$ and $p_i = \lim n_i/(n_1 + n_2)$ $(i = 1,2)$ as $\min (n_1,n_2) \to \infty$. It was shown by Fix and Hodges (1951) and DasGupta and Lin (1977) that

$$\alpha_1^* = \alpha_2^* = \int_{-\infty}^{\infty} p_2 f_1(x) f_2(x) dx / \{p_1 f_1(x) + p_2 f_2(x)\}$$

$$\alpha_3^* = \alpha_2^* + \int_{-\infty}^{\infty} \frac{p_1 p_2 f_1(x) f_2(x) \cdot \{p_2 f_2(x) - p_1 f_1(x)\}}{\{p_1 f_1(x) + p_2 f_2(x)\}^3} f_1(x) dx .$$

In this paper we have studied the finite-sample performances of these rules by estimating α based on samples from sets of two given populations.

2. The Experiment. Different steps of our simulation study are given below.

(i) Two known but different univariate distributions F_1 and F_2 are chosen.

(ii) Random samples of sizes n_1 and n_2 from F_1 and F_2, respectively, are obtained; these samples are called training samples.

(iii) A random sample of size n_0 from $F_0 = F_1$ is obtained. We call this a test sample.

(iv) For each observation in the test sample a given classification rule δ (one of the above three rules) is applied and let n_{02} be the number of the observations in the test sample which are classified by δ

into F_2 . Let $\hat{\alpha}(\delta) = n_{02}/n_0$ be the proportion of test samples misclassified into F_2 .

(v) Steps (ii)-(iv) are repeated r times for new training and test samples keeping n_1, n_2 and n_0 fixed.

(vi) The mean and the standard error of the mean based on r values of $\hat{\alpha}(\delta)$ thus obtained are recorded.

(vii) Steps (ii)-(vi) are repeated for different values of n_1, n_2 and r .

(viii) F_2 is characterized by a parameter θ . For different values of θ steps (i)-(vii) are repeated.

Our choices are given in the following table.

F_1	F_2	Parameters	$n_1=n_2$	n_0	r
N(0,1)	N(θ,1)	θ=0, $\pm$1, $\pm$2, 3	25 100	100 400	20 4
N(0,1)	N(0,θ)	θ=2, 3, 1/2, 1/3	25 100	100 400	20 4
e^{-x} (density)	$\theta e^{-\theta x}$	θ=1, 2, 3, 4, 1/2, 1/3, 1/4, 1/8	100	100	20
Cauchy (0,1)	Cauchy (θ,1)	θ=0, $\pm$1, $\pm$2, $\pm$3	25 100	100 400	20 4

Samples are generated by a library subroutine available on the CDC 6400 at the University of Minnesota.

Note 1. In the following tables "Half" refers to taking one-half the number of ties to count as misclassified and "R-half" refers to resolving the ties by the use of uniform random number generator.

Note 2. In some of the following tables EPMC denotes an estimate of the asymptotic PMC $(\alpha_1^* = \alpha_2^*)$ of the 1-NN and 1-RNN rules. These are derived by the method of runs as suggested in Das Gupta and Lin (1977).

3. Tables

Table 3.1

Proportion of test sample misclassified into π_2.

$F_1 = N(0,1)$, $F_2 = N(\theta,1)$; $n_1 = n_2 = 25$, $n_0 = 100$, $r = 20$.

Optimal (assuming θ is known and for minimax rule) PMC is $\Phi(-|\theta|/2)$.

θ \ Rule	1NN		RNN			2-RNN			Opt. Exp't.
	MEAN	s.e.		MEAN	s.e.		MEAN	s.e.	PMC
$\theta = 0$	.479	.017	Half Rhalf	.479 .485	.013 .016	Half Rhalf	.479 .484	.014 .015	.500
$\theta = 1$	.374	.018	Half Rhalf	.381 .374	.014 .016	Half Rhalf	.343 .340	.021 .021	.308
$\theta = -1$	.426	.020	Half Rhalf	.426 .432	.014 .017	Half Rhalf	.421 .425	.025 .024	.308
$\theta = 2$	.195	.018	Half Rhalf	.194 .196	.018 .018	Half Rhalf	.165 .164	.017 .018	.159
$\theta = -2$	.245	.020	Half Rhalf	.254 .251	.018 .018	Half Rhalf	.258 .255	.019 .018	.159
$\theta = 3$	.086	.012	Half Rhalf	.089 .084	.012 .011	Half Rhalf	.062 .061	.010 .009	.067
$\theta = -3$	.105	.013	Half Rhalf	.114 .113	.012 .011	Half Rhalf	.119 .118	.015 .015	.067

Table 3.2

Proportion of test sample misclassified into π_2 .

$F_1 = N(0,1)$, $F_2 = N(\theta,1)$; $n_1 = n_2 = 100$, $n_0 = 400$, $r = 4$.

θ \ Rule	1NN		RNN			EPMC	2-RNN			Opt. Exp't.
	MEAN	s.d.		MEAN	s.d.			MEAN	s.d.	PMC
$\theta = 0$	.490	.018	Half Rhalf	.482 .475	.008 .006	.48	Half Rhalf	.509 .501	.014 .016	.500
$\theta = 1$	.415	.010	Half Rhalf	.398 .404	.014 .024	.36	Half Rhalf	.351 .358	.009 .024	.308
$\theta = -1$	.402	.010	Half Rhalf	.394 .397	.007 .007	.38	Half Rhalf	.347 .344	.025 .024	.308
$\theta = 2$	.208	.010	Half Rhalf	.210 .208	.010 .009	.22	Half Rhalf	.200 .199	.011 .012	.159
$\theta = -2$	.209	.012	Half Rhalf	.213 .215	.008 .009	.22	Half Rhalf	.197 .200	.013 .014	.159
$\theta = 3$	.088	.011	Half Rhalf	.083 .082	.009 .007	.10	Half Rhalf	.065 .066	.005 .006	.007
$\theta = -3$	.104	.012	Half Rhalf	.101 .107	.008 .013	.09	Half Rhalf	.088 .094	.012 .014	.007

Table 3.3.

Proportion of test sample misclassified into π_2 .

$F_1 = N(0,1)$, $F_2 = N(0,\theta)$; $n_1 = n_2 = 25$, $n_0 = 100$. $r = 20$.

θ \ Rule	1NN		RNN		2-RNN	
	MEAN	s.e.	MEAN	s.e.	MEAN	s.e.
$\theta = 2.0$	.375	.009	Half .394 Rhalf .393	.008 .010	Half .353 Rhalf .355	.014 .015
$\theta = 3.0$	.399	.014	Half .346 Rhalf .337	.013 .013	Half .293 Rhalf .295	.019 .018
$\theta = .5$	.417	.017	Half .438 Rhalf .337	.015 .018	Half .461 Rhalf .460	.020 .021
$\theta = 1/3$	.359	.022	Half .376 Rhalf .380	.018 .019	Half .393 Rhalf .391	.019 .019

Table 3.4

Proportion of test sample misclassified into π_2 .

$F_1 = N(0,1)$, $F_2 = N(0,\theta)$; $n_1 = n_2 = 100$, $n_0 = 400$, $r = 4$.

θ \ Rule	1NN		RNN		EPMC	2-RNN	
	MEAN	s.e.	MEAN	s.e.		MEAN	s.e.
$\theta = 2.0$	.435	.022	Half .424 Rhalf .426	.022 .025	.36	Half .395 Rhalf .396	.027 .028
$\theta = 3.0$	.333	.012	Half .338 Rhalf .336	.010 .011	.32	Half .295 Rhalf .296	.012 .011
$\theta = .5$	.397	.062	Half .405 Rhalf .407	.011 .013	.38	Half .409 Rhalf .408	.006 .005
$\theta = 1/3$	.339	.021	Half .352 Rhalf .354	.020 .021	.35	Half .360 Rhalf .361	.029 .030

Table 3.5

Proportion of test sample misclassified into π_2 .

$f_1(x) = e^{-x}$, $f_2(x) = \theta e^{-\theta x}$; $n_1 = n_2 = n_0 = 100$, $r = 4$.

θ \ Rule	1NN		RNN		EPMC	2-RNN	
	MEAN	s.e.	MEAN	s.e.		MEAN	s.e.
$\theta = 1$	.508	.016	Half .509 Rhalf .523	.013 .016	.47	Half .503 Rhalf .517	.013 .015
$\theta = 2$	.442	.015	Half .434 Rhalf .438	.014 .017	.38	Half .442 Rhalf .444	.016 .016
$\theta = 3$	.402	.014	Half .388 Rhalf .387	.011 .011	.36	Half .394 Rhalf .387	.013 .014
$\theta = 4$	.335	.009	Half .330 Rhalf .336	.007 .008	.32	Half .327 Rhalf .330	.009 .009
$\theta = .5$	.453	.010	Half .453 Rhalf .458	.009 .013	.38	Half .430 Rhalf .430	.010 .014
$\theta = 1/3$	.410	.011	Half .395 Rhalf .386	.008 .009	.36	Half .346 Rhalf .335	.010 .010
$\theta = 1/4$	.354	.015	Half .364 Rhalf .372	.012 .013	.32	Half .290 Rhalf .292	.013 .013
$\theta = 1/8$	.247	.014	Half .248 Rhalf .259	.012 .014	.22	Half .181 Rhalf .185	.011 .010

Table 3.6

Proportion of test sample misclassified into π_2.

F_1 = Cauchy(0,1), F_2 = Cauchy(θ,1); $n_1 = n_2 = 25$, $n_0 = 100$, $r = 20$.

θ \ Rule	1NN		RNN			2-RNN		
	MEAN	s.e.		MEAN	s.e.		MEAN	s.e.
$\theta = 0$	.473	.018	Half	.430	.015	Half	.488	.027
			Rhalf	.493	.018	Rhalf	.505	.029
$\theta = 1$	.406	.022	Half	.418	.022	Half	.397	.031
			Rhalf	.408	.025	Rhalf	.395	.033
$\theta = -1$	.398	.016	Half	.410	.012	Half	.389	.021
			Rhalf	.410	.013	Rhalf	.385	.022
$\theta = 2$	.288	.021	Half	.297	.021	Half	248	.027
			Rhalf	.288	.021	Rhalf	.238	.028
$\theta = -2$	.247	.012	Half	.264	.012	Half	.248	.017
			Rhalf	.276	.015	Rhalf	.252	.019
$\theta = 3$	.161	.020	Half	.168	.017	Half	.103	.017
			Rhalf	.161	.018	Rhalf	.099	.017
$\theta = -3$	.153	.015	Half	.156	.013	Half	.130	.014
			Rhalf	.154	.013	Rhalf	.125	.014

Table 3.7

Proportion of test sample misclassified into π_2 .

F_1 = Cauchy(0,1), F_2 = Cauchy(θ,1); $n_1 = n_2 = 100$, $n_0 = 400$, $r = 4$.

θ \ Rule	1NN		RNN			2-RNN		
	MEAN	s.e.		MEAN	s.e.		MEAN	s.e.
$\theta = 0$	.494	.015	Half Rhalf	.514 .529	.013 .014	Half Rhalf	.506 .512	.017 .021
$\theta = 1$	.411	.010	Half Rhalf	.426 .446	.009 .018	Half Rhalf	.381 .390	.018 .017
$\theta = -1$	.457	.029	Half Rhalf	.446 .454	.033 .025	Half Rhalf	.394 .393	.028 .025
$\theta = 2$	.284	.007	Half Rhalf	.278 .283	.008 .009	Half Rhalf	.217 .219	.033 .024
$\theta = -2$	.152	.016	Half Rhalf	.318 .321	.022 .015	Half Rhalf	.254 .257	.014 .010
$\theta = 3$	.152	.016	Half Rhalf	.154 .417	.015 .012	Half Rhalf	.088 .087	.018 .014
$\theta = -3$	.204	.034	Half Rhalf	.199 .198	.032 .034	Half Rhalf	.105 .103	.011 .012

4. Concluding Remarks. For all the three rules considered, it seems that $\hat{\alpha}_1$ has a definite tendency to decrease as θ moves away (in either direction) from its value under F_1.

For small $n_1 = n_2$ there is not any marked difference in performances of these three rules although the 2-RNN rule may be a bit better. However, for large $n_1 = n_2$ the 2-RNN rule seem to have markedly better performance except for the cases $N(0,1)$ vs. $N(0,\theta)$, $\theta < 1$. This report is the first empirical study on the performances of 1NN and RNN rules, although a more detailed study especially on multi-stage RNN rules is called for.

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